Supporting Information

Design and Synthesis of a new Class of selective Integrin α5β1 Antagonists

Roland Stragies, Frank Osterkamp, Gunther Zischinsky, Doerte Vossmeyer, Holger Kalkhof, Ulf Reimer and Grit Zahn*

Content

Experimental procedures for microsome stability assay, cell based assay and analytical data and experimental procedures for the compounds **12a**, **16a-c**, **19a**, **19c-k** and **17**. Table of purity and HPLC analysis for the target compounds **1**, **7a-e**, **12a-c** and **19a-k**.

Microsomal stability assay

The stability of the compounds in human microsomal preparations was determined as described in Kunz, W.; Gieschen, H. *Drug. Metab. Dispos.* **1998**, *26*, 1120.

Cell adhesion assay

Cell adhesion assays were performed with human embryonal kidney cells HEK293 (DSMZ, Braunschweig, Germany). 96 well plates were coated with 10 µg/ml fibronectin (Chemicon, Europe, Hampshire, UK) and blocked with 1% BSA. Cells were grown to 80% confluence in DMEM (Biochrome AG, Berlin ,Germany) supplemented with 10% FCS and 2 mM glutamine and detached with cell dissociation solution (Sigma-Aldrich, Taufkirchen, Germany). Cells were incubated for 30 min in HEPES buffered saline with 2 mM EDTA (25

mM HEPES, 150 mM NaCL, 2 mM EDTA, pH7.4). Cells were transferred to EDTA-free buffer supplemented with 50 nM PMA and 2 mM $MgCl_2$. Small molecule integrin antagonists were added to cells and DMSO concentrations were adjusted. $0.7x10^4$ cells/well were plated on fibronectin-coated plates for 1 h at 37°C. Plates were washed and adherent cells were fixed with 5% glutaraldeyde for 30 min, rinsed and stained with 0.1% crystal violet for 1 h. After rinsing plates 10% acetic acid was added and plates were analyzed at 570 nm with a Spectra Max® M5 microplate reader (Molecular Devices, Sunnyvale, CA, USA). IC_{50} values were determined using the XL-Fit software.

Experimental

2*S*,4*R*,20*S*-4-{[2-carboxy-2-(2,4,6-trimethyl-benzenesulfonylamino)-ethylcarbamoyl]-methoxy}-2-[(4-methoxy-pyridin-2-ylamino)-methyl]-pyrrolidine-1-carboxylic acid benzyl ester (12a). Compound **12a** was obtained in 55% over all yield. NMR-^{1}H (DMSO-D_6): (partial signal doubling due to rotameres) δ = 12.95 (s, broad, 1H), 8.31 (s, broad, 1H), 7.93 (d, 1H, *J* = 8.8), 7.86 (d, 1H, *J* = 7.3), 7.71 (t, 1H, *J* = 5.9), 7.39 - 7.22 (m, 4H), 6.95 (s, 2H), 6.58 (m, 1H), 6.55 (d, 1H, *J* = 7.3), 5.09 (s, 2H), 4.19 (m, 1H), 4.10 (m, 2H), 3.92 3.85 - 3.39 (m, 11H), 3.15 (m, 1H), 2.51 (s, 3H), 2.49 (m, 6H), 2.18 (m, 1H), 1.88(m, 1H). LCMS: *m/z*: 684.2 [MH^+].

General procedure for the synthesis of compounds 16a-c.

Compounds 16a-c were synthesized according to the protocols for the synthesis of 4 described under general procedure A. Synthesis of 2*S*,4*R*-{1-(3,3-dimethyl-butyryl)-5-[(4-methoxy-pyridin-2-ylamino)-methyl]-pyrrolidin-3-yloxy}-acetic acid (16a). Compound **16a** was obtained in 43% over all yield. NMR-^{1}H (DMSO-D_6): (partial signal doubling due to rotameres) δ = 13.13 (s, broad, 1H), 8.42 (s, 1H), 7.87 (d, 1H, *J* = 5.8), 7.38 - 7.23 (m, 2H), 6.58 (s, 1H), 6.54 (d, 1H, *J* = 5.8), 5.09 (d, 2H, *J* = 3.7), 5.04 (dd, 1H, *J* = 6.4, *J*

= 12.5), 4.17 (s, 1H), 4.05 (s, 3H), 3.65 (m, 2H), 3.43 (m, 2H), 2.18 (m, 1H), 1.89 (m, 1H), 0.93 (s, 9H). NMR-^{13}C (DMSO-D_6): partial signal doubling due to rotameres) δ = 171.5 (Cq), 158.7 (Cq), 155.0 (Cq), 136.6 (Cq), 128.3 (CH), 127.7 (CH), 127.3 (CH), 104.1 (CH), 76.9 (CH), 66.3 (CH_2), 66.1 (CH_2), 65.5 (CH_2), 56.7 (CH_3), 51.7 (Cq), 44.2 (CH_2), 34.4 (CH_2) 29.6 (CH_3). LCMS: m/z: 380.6 [MH^+].

Synthesis of 2*S*,4*R*-{1-(3,3-dimethyl-butyryl)-5-[(pyridin-2-ylamino)-methyl]-pyrrolidin-3-yloxy}-acetic acid (16b). Compound **16b** was obtained in 63% over all yield. NMR-^{1}H (DMSO-D_6): (partial signal doubling due to rotameres) δ = 12.70 (s, broad, 1H), 8.72 (s, 1H), 7.97 (d, 1H, *J* = 5.7), 7.90 (t, 1H, *J* = 8.0), 7.12 (d, 1H, *J* = 8.7), 6.84 (t, 1H, *J* = 6.5), 4.21 (m, 2H), 4.04 (s, 2H), 3.67 (d, 1H, *J* = 10.9), 3.58 (dd, 1H, *J* = 4.3, *J* = 11.7), 3.56 (m, 1H), 3.42 (m, 1H), 2.24 (d, 1H, *J* = 13.9), 2.22 (d, 1H, *J* = 14.7), 2.14 (m, 1H) 2.12 (dt, 1H, *J* = 13.9, *J* = 5.8), 1.96 (m, 1H), 0.97 (s, 9H). NMR-^{13}C (DMSO-D_6): partial signal doubling due to rotameres) δ = 178.6 (CH), 171.5 (Cq), 158.8 (Cq), 153.4 (Cq), 143.0 (CH), 142.6 (CH), 136.8 (CH), 112.0 (CH), 77.0 (CH), 65.6 (CH_2), 53.9 (Cq), 52.7 (CH_2), 46.1 (CH_2), 44.2 (CH_2), 34.5 (CH_2), 29.5 (CH_3). LCMS: m/z: 350.8 [MH^+].

Synthesis of 2*S*,4*R*-{4-carboxymethoxy-2-[(4-methoxy-pyridin-2-ylamino)-methyl]-pyrrolidine-1-carboxylic acid benzyl ester (16c). Compound **16c** was obtained in 41% over all yield. NMR-^{1}H (DMSO-D_6): (partial signal doubling due to rotameres) δ = 13.15 (s, broad, 1H), 8.38 (s, 1H), 7.90 (s, 1H), 7.84 (d, 1H, *J* = 7.3), 7.41 - 7.26 (m, 5H), 6.57 (s, 1H), 6.51 (d, 1H, *J* = 7.3), 6.34 (d, 1H, *J* = 2.9), 5.08 (d, 1H, *J* = 2.1), 5.03 (m, 1H), 4.17 (m, 1H), 4.02 (s, 3H), 3.82 (m, 1H), 3.68 (m, 2H), 3.50 (m, 2H), 2.18 (m, 1H), 1.88 (m, 1H). NMR-^{13}C (DMSO-D_6): partial signal doubling due to rotameres) δ = 171.5 (Cq), 158.7 (Cq), 156.0 (Cq), 155.2 148.5 (CH), 148.3 (CH), 142.2 (Cq), 137.2 (CH), 137.7 (Cq), 128.3 (CH), 127.8 (CH),

127.3 (CH), 118.9 (CH_2), 104.2 (CH), 92.3 (CH), 66.3 (CH_2), 66.1 (CH_2), 65.5 (CH_2), 54.4 (CH_3), 51.8 (CH_2). LCMS: m/z: 416.2 [MH^+].

2*S*,4*R*,20*S*-4-[(2-benzenesulfonylamino-2-carboxy-ethylcarbamoyl)-methoxy]-2-(pyridin-2-ylaminomethyl)-pyrrolidine-1-carboxylic acid benzyl ester (19a). NMR-^{1}H (DMSO-d_6): (partial signal doubling due to rotameres) δ = 8.25 (s, broad, 1H), 8.18 (d, 1H, *J* = 8.3), 7.98-7.67 (m, 5H), 7.67-7.48 (m, 4H), 7.35 (m, 6H), 7.02 (dm, 1H, *J* = 8.3), 6.81 (tm, 1H, *J* = 5.9), 5.08 (s, 1H), 4.10 (m, 3H), 3.95-3.34 (m, 6H), 3.14 (m, 1H), 2.17 (m, 1H), 1.91 (m, 1H). LCMS: *m/z*: 612.5 [MH^+].

2*S*,4*R*,20*S*-4-{[2-carboxy-2-(2,4,6-trimethyl-benzoylamino)-ethylcarbamoyl]-methoxy}-2-(pyridin-2-ylaminomethyl)-pyrrolidine-1-carboxylic acid benzyl ester (19c). NMR-^{1}H (DMSO-D_6): (partial signal doubling due to rotameres) δ = 13.80 (s, broad, 1H), 8.75 (d, 1H, *J* = 7.3), 8.43 (m, 1H), 7.91 (m, 1H), 7.75 (t, 1H, *J* = 5.8), 7.40 - 7.30 (m, 4H), 7.15 (d, 1H, *J* = 7.3), 6.86 (t, 1H, *J* = 6.6), 6.80 (s, 1H), 5.06 (s, H), 5.02 (m, 1H), 4.49 (m, 1H), 4.16 (m, 1H), 4.12 (m, 1H), 3.85 (s, 2H), 3.81 - 3.47 (m, 10H), 3.38 (m, 1H), 2.21 (s, 3H), 2.16 (s, 6H), 1.94 (m, 1H). LCMS: *m/z*: 619.1 [MH^+].

2*S*,4*R*,20*S*-4-({2-carboxy-2-[(1-methyl-cyclohexanecarbonyl)-amino]-ethylcarbamoyl}-methoxy)-2-(pyridin-2-ylaminomethyl)-pyrrolidine-1-carboxylic acid benzyl ester (19d). NMR-^{1}H (DMSO-D_6): (partial signal doubling due to rotameres) δ = 13.26 (s, broad, 1H), 8.28 (s, broad, 1H), 7.94 (d, 1H, *J* = 5.1), 7.90 (m, 1H), 7.84 (m, 1H), 7.81 (m, 1H), 7.62 (d, 1H, *J* = 7.3), 7.39 - 7.29 (m, 7H), 7.04 (m, 1H), 6.82 (m, 1H), 5.07 (s, 1H), 5.02 (m, 1H), 4.17 (m, 1H), 4.12 (m, 2H), 3.84 (m, 1H), 3.75 - 3.35 (m, 10H), 2.18 (m, 1H), 1.90 (m, 2H), 1.40 - 1.07 (m, 5H), 0.99 (s, 3H). LCMS: *m/z*: 595.8 [MH^+].

2*S*,3*R*,5*S*-3-{2-[1-(3,3-dimethyl-butyryl)-5-(pyridin-2-ylaminomethyl)-pyrrolidin-3-yloxy]-acetylamino}-2-(2,4,6-trimethyl-benzoylamino)-propionic acid (19e). **N**MR-^{1}H (DMSO-D_6): (partial signal doubling due to rotameres) δ = 8.93 (s, broad, 1H), 8.85 (d, 1H, *J* = 7.3), 7.96 (m, broad, 2H), 7.75 (t, 1H, *J* = 5.8), 7.11 (d, 1H, *J* = 6.8), 6.88 (t, 1H, J = 8.8), 6.81 (s, broad, 2H), 4.50 (m, broad, 1H), 4.21 (m, broad, 2H), 3.89 (d, 2H, *J* = 2.9), 3.64 (m, broad, 4H), 3.41 (m, broad, 1H), 2.04 (m, broad, 1H), 2.22 (s, 3H), 2.17 (s, 6H), 0.97 (s, 9H). LCMS: *m/z*: 582.7 [MH^+].

2*S*,3*R*,5*S*-3-{2-[1-(3,3-dimethyl-butyryl)-5-(pyridin-2-ylaminomethyl)-pyrrolidin-3-yloxy]-acetylamino}-2-[(1-methyl-cyclohexanecarbonyl)-amino]-propionic acid (19f). NMR-^{1}H (DMSO-D_6): (partial signal doubling due to rotameres) δ = 13.84 (s, broad, 1H), 8.88 (s, broad, 1H), 7.95 (m, 2H), 7.84 (t, 1H, *J* = 6.6), 7.69 (d, 1H, *J* = 7.3), 7.19 (m, 1H), 6.86 (d, 1H, *J* = 6.6), 4.26 (m, 1H), 4.19 (m, 2H), 3.88 (s, 3H), 3.71 (dm, 1H, *J* = 11.0), 3.61 (dd, 1H, *J* = 5.1, *J* = 11.7), 3.56 – 3.49 (m, 6H), 3.39 (m, 1H), 2.25 (d, 1H, *J* = 14.7), 2.17 (m, 1H), 2.12 (d, 1H, *J* = 14.7), 2.00 (m, 1H), 1.91 (m, 2H), 1.40 (m, 4H), 1.28 (m, 1H), 1.24 - 1.09 (m, 3H), 1.01 (s, 3H), 0.97 (m, 9H). LCMS: *m/z*: 560.6 [MH^+].

2*S*,3*R*,5*S*-4-{[2-carboxy-2-(2,4,6-trimethyl-benzoylamino)-ethylcarbamoyl]-methoxy}-2-[(4-methoxy-pyridin-2-ylamino)-methyl]-pyrrolidine-1-carboxylic acid benzyl ester (19g). NMR-^{1}H (DMSO-D_6): (partial signal doubling due to Cbz-rotameres) δ = 13.31 (s, broad, 1H), 8.45 (m, broad, 2H), 7.87 (d, 1H, *J* = 7.3), 7.76 (t, 1H, *J* = 5.8), 7.35 (s, 4H), 7.29 (s, 2H), 6.80 (s, 2H), 6.62 (s, 1H), 6.55 (d, 1H, *J* = 7.3), 5.09 (m, broad, 3H), 4.52 (m, broad, 1H), 4.17 (m, broad, 1H), 4.08 (m, broad, 1H), 3.86 (s, 3H), 3.60 (m, broad, 4H), 3.53 (m, broad, 1H), 3.39 (m, broad, 1H), 2.22 (s, 3H), 2.16 (s, 6H), 1.96 (m, broad, 1H). LCMS: *m/z*: 648.5 [MH^+].

2*S*,3*R*,20*S*-3-(2-{1-(3,3-dimethyl-butyryl)-5-[(4-methoxy-pyridin-2-ylamino)-methyl]-pyrrolidin-3-yloxy}-acetylamino)-2-(2,4,6-trimethyl-benzenesulfonylamino)-propionic acid (19h). NMR-^{1}H (DMSO-D_6): (partial signal doubling due to rotameres) δ = 13.30 (s, broad, 1H), 8.55 (s, broad, 1H), 7.97 (d, 1H, *J* = 9.5), 7.87 (d, 1H, *J* = 7.3), 7.71 (t, 1H, *J* = 5.6), 6.97 (s, 2H), 6.79 (m, 2H), 6.53 (dd, 1H, *J* = 2.2, *J* = 7.3), 4.15 (m, 2H), 3.94 (s, 3H), 3.84 (m, 3H), 3.77 (d, 1H, *J* = 17.6), 3.65 (m, 2H), 3.55 (m, 1H), 3.44 (m, 2H), 3.17 (ddd, 1H, *J* = 5.9, *J* = 8.0, *J* = 13.9), 2.52 (s, 6H), 2.49 (s, 3H), 2.23 (m, 3H), 2.15 (d, 1H, *J* = 13.9), 2.13 (m, 1H), 2.00 (dt, 1H, *J* = 5.9, *J* = 13.2), 0.99 (s, 9H). LCMS: *m/z*: 648.7 [MH^+].

2*S*,3*R*,5*S*-3-(2-{1-(3,3-dimethyl-butyryl)-5-[(4-methoxy-pyridin-2-ylamino)-methyl]-pyrrolidin-3-yloxy}-acetylamino)-2-(2,4,6-trimethyl-benzoylamino)-propionic acid (19i). NMR-^{1}H (DMSO-D_6): (partial signal doubling due to rotameres) δ = 13.42 (s, broad, 1H), 8.49 (m, broad, 2H), 8.45 (d, 1H, *J* = 7.3), 7.89 (d, 1H, *J* = 7.3), 7.75 (t, 1H, *J* = 6.3), 6.81 (s, 3H), 6.54 (dd, 1H, *J* = 2.4, *J* = 7.3), 4.50 (m, broad, 1H), 4.20 (m, broad, 2H), 3.96 (s, 3H), 3.88 (m, broad, 2H), 3.64 (m, broad, 2H), 3.58 (m, broad, 2H), 3.42 (m, broad, 2H), 2.22 (s, 3H), 2.17 (s, 6H), 2.15 (s, 3H), 2.05 (m, broad, 1H), 0.99 (s, 9H). LCMS: *m/z*: 612.7 [MH^+].

2*S*,3*R*,5*S*-4-({2-carboxy-2-[(1-methyl-cyclohexanecarbonyl)-amino]-ethylcarbamoyl}-methoxy)-2-[(4-methoxy-pyridin-2-ylamino)-methyl]-pyrrolidine-1-carboxylic acid benzyl ester (19j). NMR-^{1}H (DMSO-D_6): (partial signal doubling due to rotameres) δ = 13.28 (s, broad, 1H), 8.45 (s, broad, 1H), 7.86 (m, 2H), 7.65 (d, 1H, *J* = 7.3), 7.37 - 7.27 (m, 5H), 6.60 (m, 1H), 6.54 (d, 1H, *J* = 7.3), 5.08 (s, 2H), 4.26 (m, 1H), 4.14 (m, 1H), 4.07 (m, 1H), 3.91 (s, 1H), 3.90 (s, 3H),3.65 - 3.34 (m, 10H), 2.20 (m, 1H), 1.92 (m, 3H), 1.39 (m, 4H), 1.25 (m, 1H), 1.22 - 1.07 (m, 3H), 0.99 (m, 3H). LCMS: *m/z*: 626.9 [MH^+].

2*S*,3*R*,5*S*-3-(2-{1-(3,3-dimethyl-butyryl)-5-[(4-methoxy-pyridin-2-ylamino)-methyl]-pyrrolidin-3-yloxy}-acetylamino)-2-[(1-methyl-cyclohexanecarbonyl)-amino]-propionic acid (19k). NMR-^{1}H (DMSO-D_6): (partial signal doubling due to rotameres) δ = 13.36 (s, broad, 1H), 8.59 (m, broad, 2H), 7.88 (d, 1H, *J* = 7.3), 7.75 (t, 1H, *J* = 5.8), 6.80 (m, broad, 1H), 6.55 (dd, 1H, *J* = 2.4, *J* = 7.3), 4.27 (m, broad, 1H), 4.19 (m, broad, 2H), 3.96 (s, 3H), 3.66 - 3.53 (m, broad, 4H), 3.41 (m, broad, 2H), 2.24 (d, 1H, *J* = 14.2), 2.13 (d, 1H, *J* = 14.2), 2.03 (m, broad, 1H), 1.94 (m, broad, 2H), 1.48- 1.08 (m, broad, 6H), 0.99 (s, 3H), 0.97 (s, 9H). LCMS: *m/z*: 590.6 [MH^+].

Synthesis of 3*S*-3-amino-2-(2,4,6-trimethyl-benzoylamino)-propionic acid tert-butyl ester (17) Compound **17** was obtained in 67% over all yield. NMR-^{1}H (DMSO-D_6): δ = 8.46 (d, 1H, *J* = 7.3), 6.85 (s, 2H), 4.26 (ddd, 1H, *J* = 4.3, *J* = 7.3, *J* = 11.7), 3.20 (s, broad, 2H), 2.88 (dd, 1H, *J* = 4.3, *J* = 13.1), 2.83 (dd, 1H, *J* = 8.0, *J* = 13.1), 2.23 (s, 3H), 2.21 (s, 6H), 1.42 (s, 9H). NMR-^{13}C (DMSO-D_6): δ = 170.2 (Cq), 169.3 (Cq), 137.1 (Cq), 135.4 (Cq), 133.8 (Cq), 127.5 (CH), 80.4 (Cq), 56.4 (CH), 43.1 (CH_2), 27.7 (CH_3), 20.6 (CH_3), 18.8(CH_3). LCMS: m/z: 307.4 [MH^+].

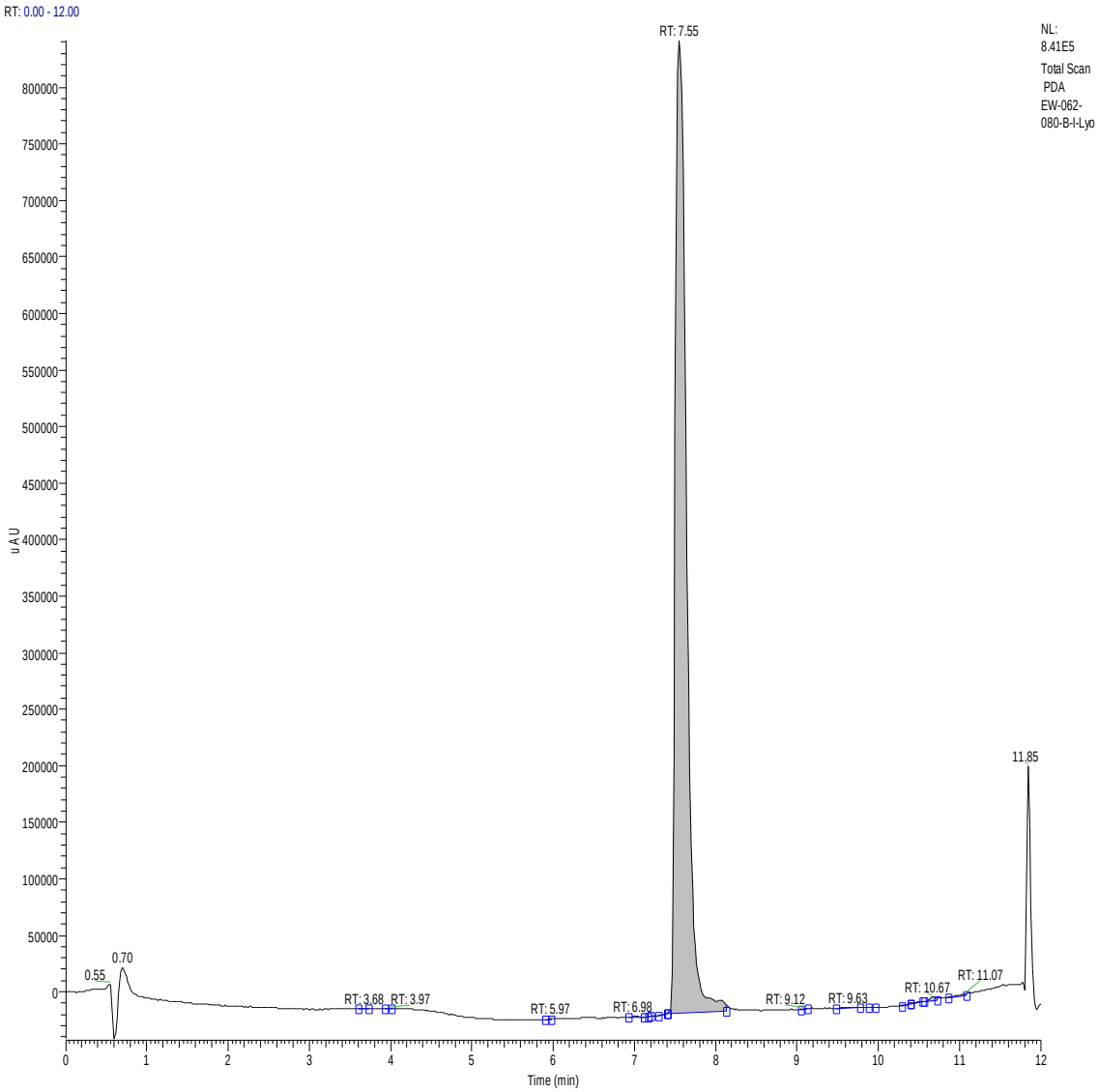
Purity of target compounds

The compounds **1**, **7a-e**, **12a-c** and **19a-k** were purified by HPLC with >95% purity (10-20 mg). The corresponding over all yields were between 15-55%. The purity was analyzed by HPLC/MS using a Surveyor HPLC combined with an LCQ classic or Advantage (all Thermo Electron, US) equipped with an ESI-source. The gradient was 5%-95% ACN/ water (0.01% TFA) in 12 minutes. Only peaks occurring between 1.00 min - 10.5 min were taken into account for the purity analysis (according to the “blank” chromatogram, page 28).

Purity

compound no.	Purity (%)

1	99.25
7a	99.00
7b	98.96
7c	98.20
7d	96.68
7e	99.51
12a	99.82
12b	99.84
12c	98.41
19a	99.37
19b	99.75
19c	99.88
19d	99.38
19e	99.28
19f	>99.9
19g	98.68
19h	98.91
19i	99.06
19j	>99.9
19k	99.82
blank	-

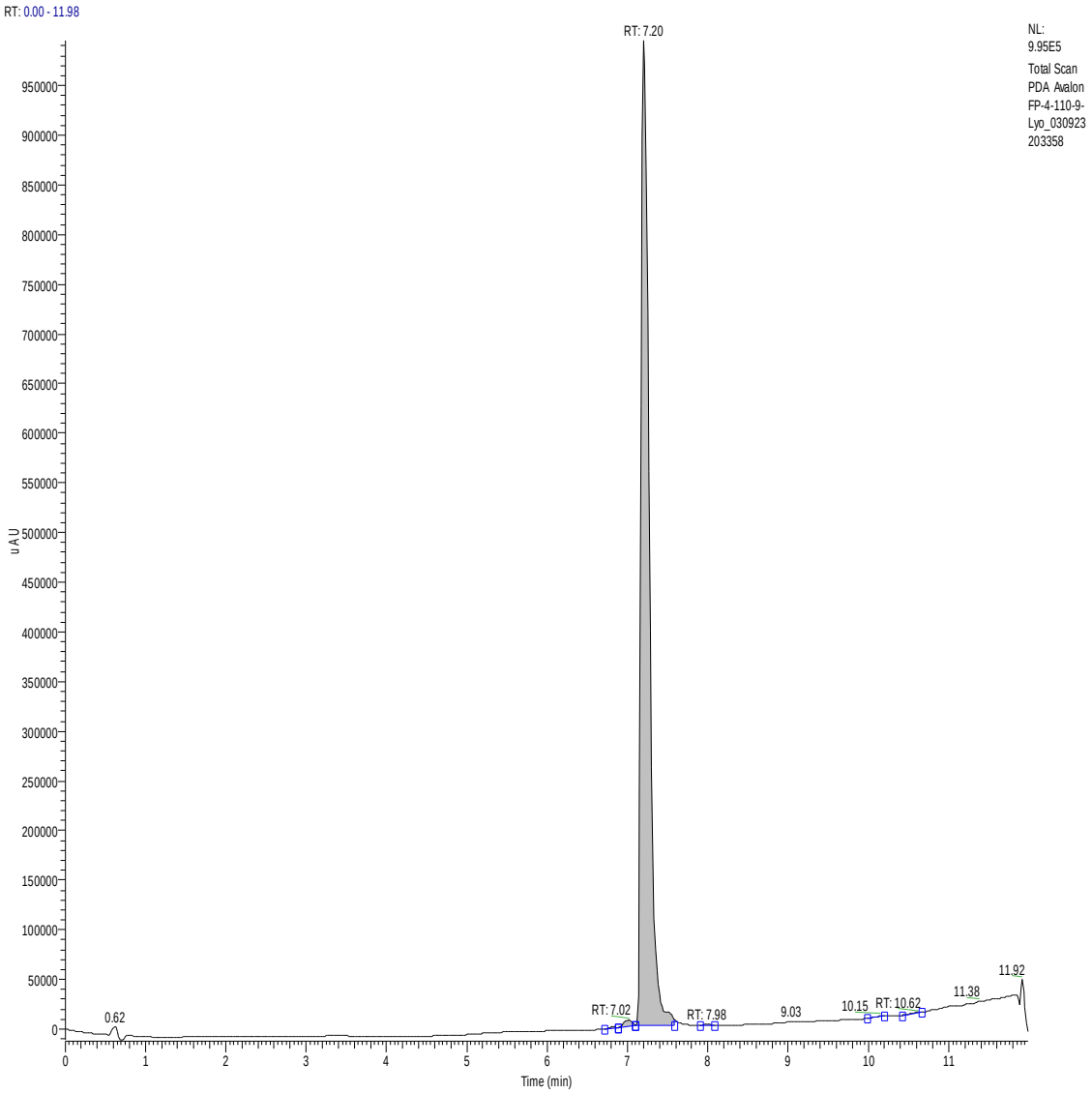


PEAK LIST

Compound 1

Number of detected peaks: 14

Apex RT	Start RT	End RT	Area	%Area
3.68	3.6	3.73	2500.5	0.03
3.97	3.93	4.02	1562.859	0.02
5.97	5.9	5.98	1659.487	0.02
6.98	6.93	7.12	5869.064	0.07
7.18	7.17	7.2	514.077	0.01
7.38	7.3	7.4	2428.538	0.03
7.55	7.42	8.13	8410541.37	99.25
9.12	9.05	9.13	1386.859	0.02
9.63	9.48	9.78	6606.115	0.08
9.9	9.88	9.97	2348.205	0.03
10.38	10.3	10.4	2890.722	0.03
10.52	10.4	10.55	6231.615	0.07
10.67	10.57	10.73	18374.756	0.22
11.07	10.87	11.08	11030.154	0.13

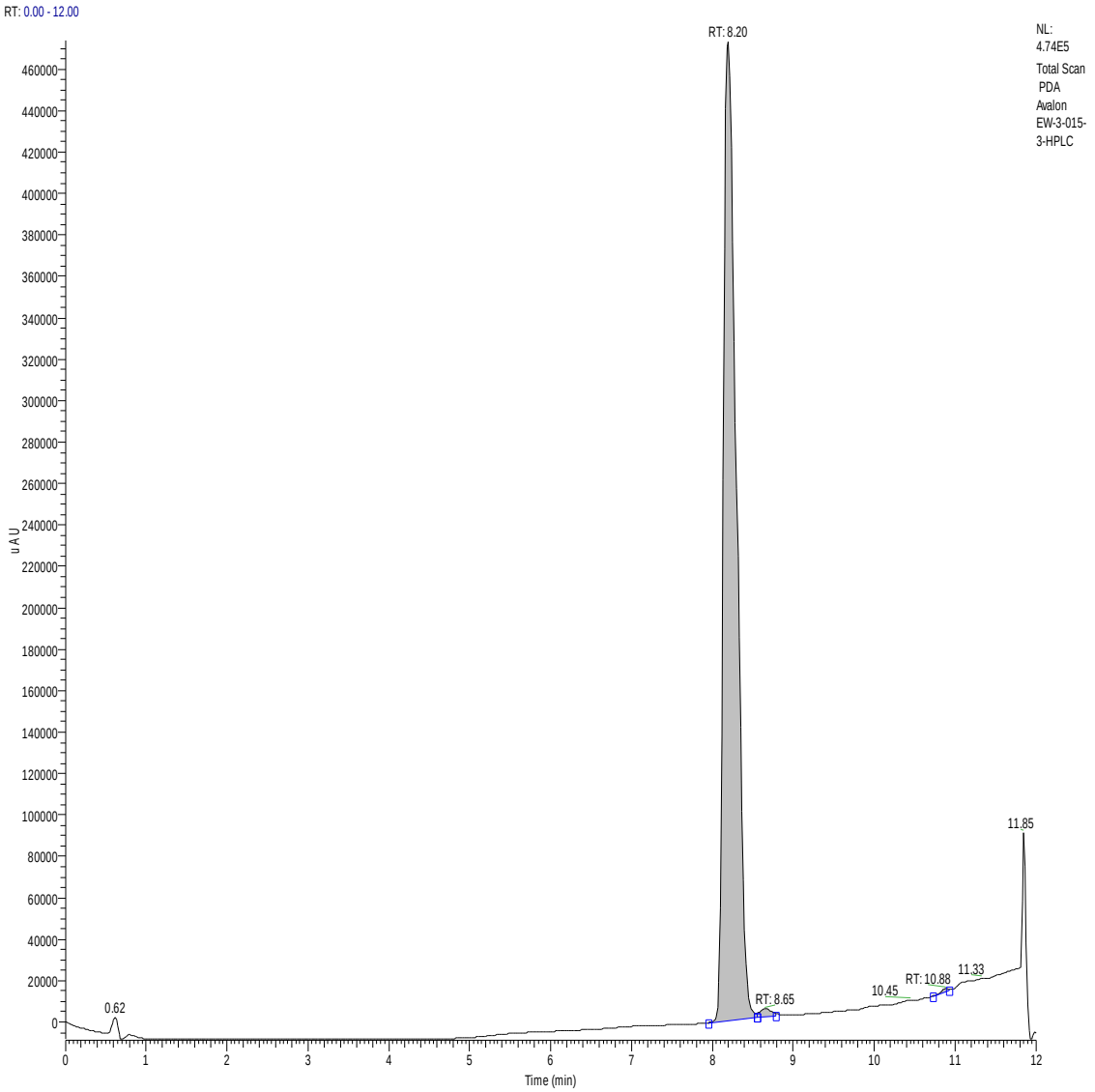


PEAK LIST

Compound 7a

Number of detected peaks: 6

Apex RT	Start RT	End RT	Area	%Area
6.82	6.72	6.88	8067.09	0.11
7.02	6.88	7.1	44054.846	0.61
7.2	7.1	7.58	7157571.49	99.00
7.98	7.9	8.08	8115.282	0.11
10.15	9.98	10.2	4647	0.06
10.62	10.42	10.67	7727.256	0.11

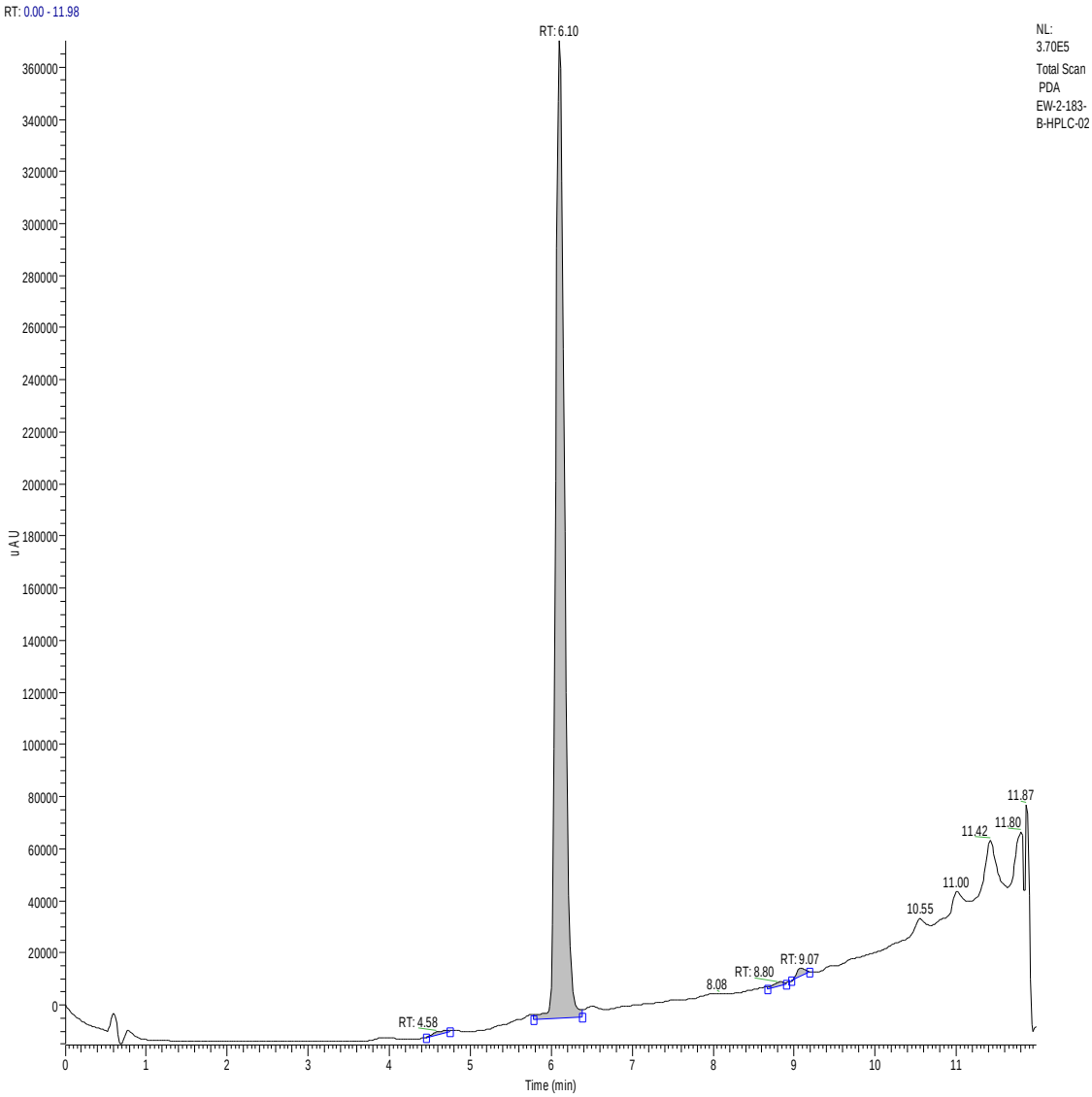


PEAK LIST

Compound 7b

Number of detected peaks: 3

Apex RT	Start RT	End RT	Area	%Area
8.2	7.95	8.55	5199271.95	98.96
8.65	8.55	8.78	43100.91	0.82
10.88	10.73	10.93	11275.577	0.21

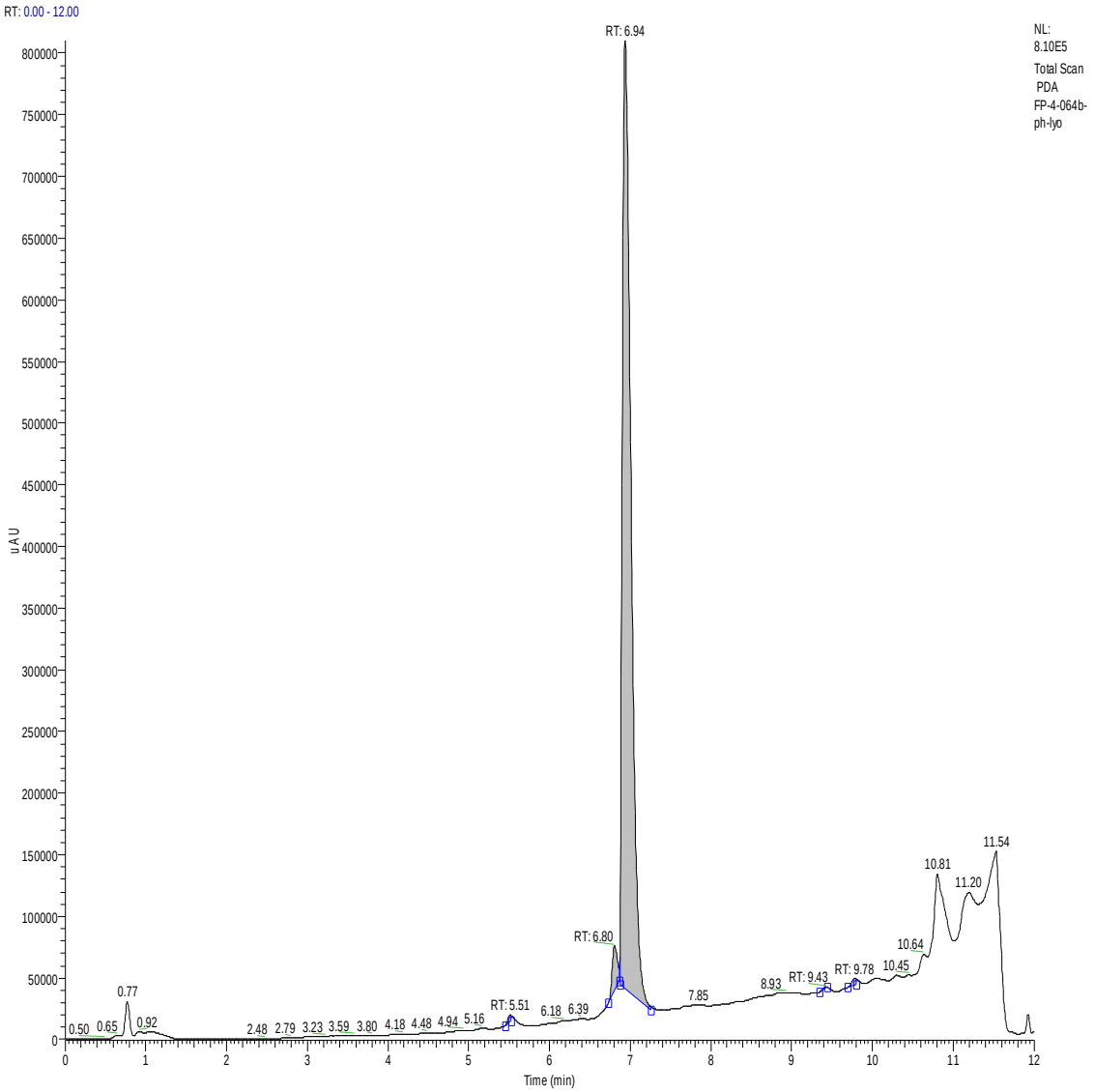


PEAK LIST

Compound 7c

Number of detected peaks: 4

Apex RT	Start RT	End RT	Area	%Area
4.58	4.45	4.75	15543.787	0.53
6.1	5.78	6.38	2869670.62	98.20
8.8	8.67	8.9	15419.795	0.53
9.07	8.97	9.18	21503.273	0.74

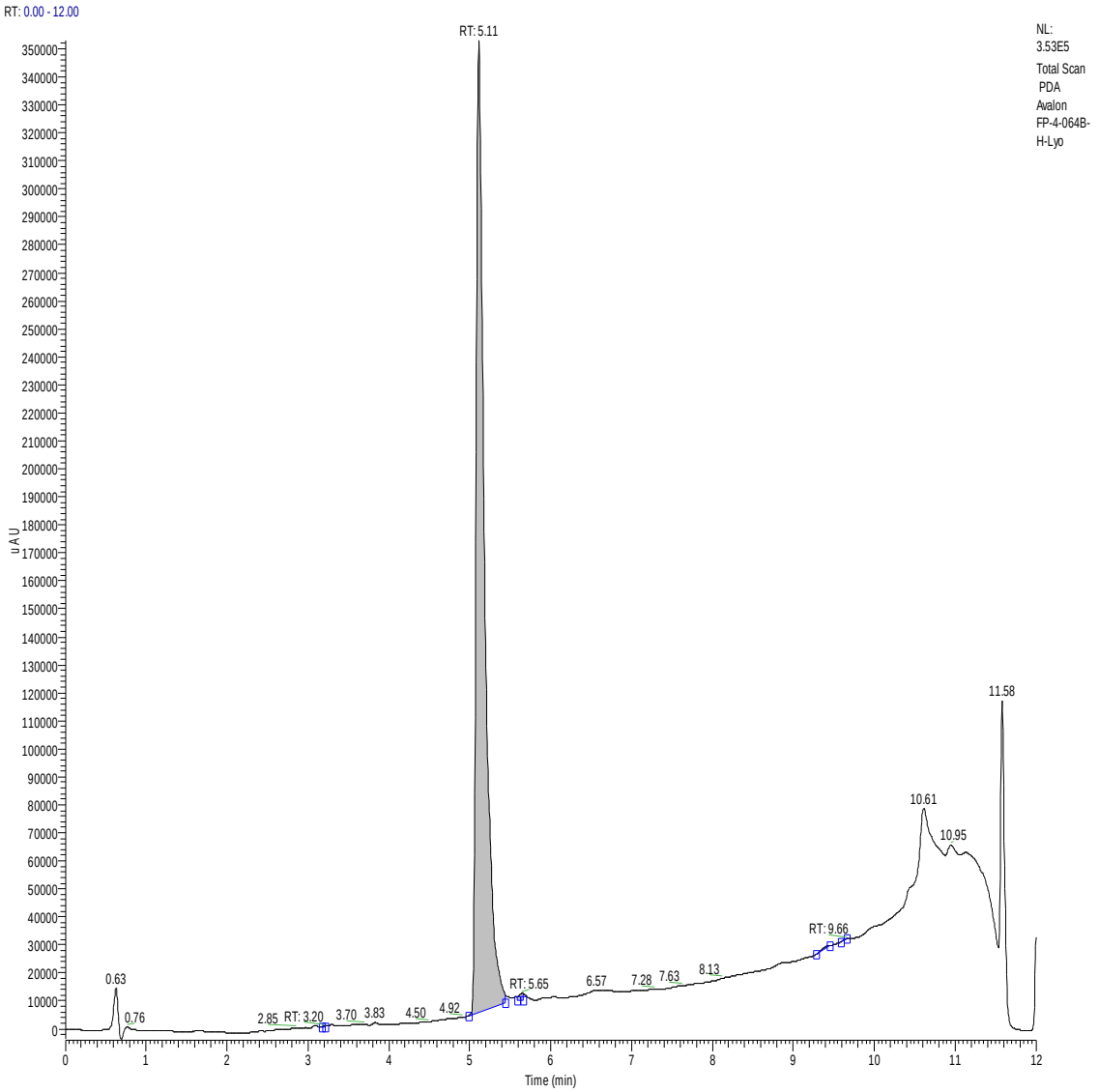


PEAK LIST

Compound 7d

Number of detected peaks: 5

Apex RT	Start RT	End RT	Area	%Area
5.51	5.45	5.53	15607.562	0.27
6.8	6.73	6.87	158476.656	2.7
6.94	6.87	7.26	5674298.36	96.68
9.43	9.35	9.44	4440.768	0.08
9.78	9.7	9.8	16401.863	0.28

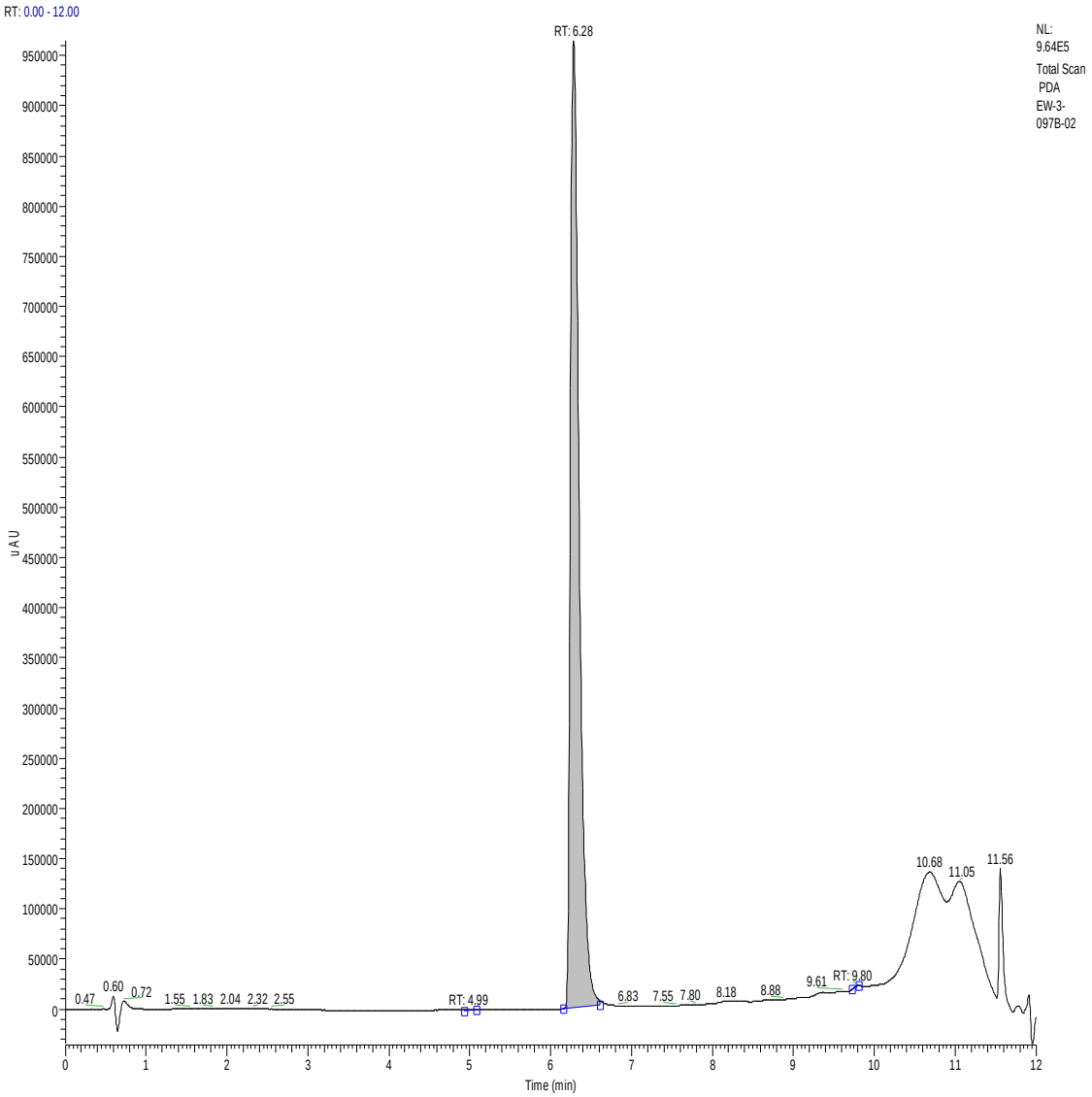


PEAK LIST

Compound 7e

Number of detected peaks: 5

Apex RT	Start RT	End RT	Area	%Area
3.2	3.17	3.22	595.055	0.02
5.11	4.99	5.45	2539123.2	99.51
5.65	5.58	5.66	7629.681	0.3
9.45	9.28	9.45	3194.125	0.13
9.66	9.59	9.67	987.192	0.04

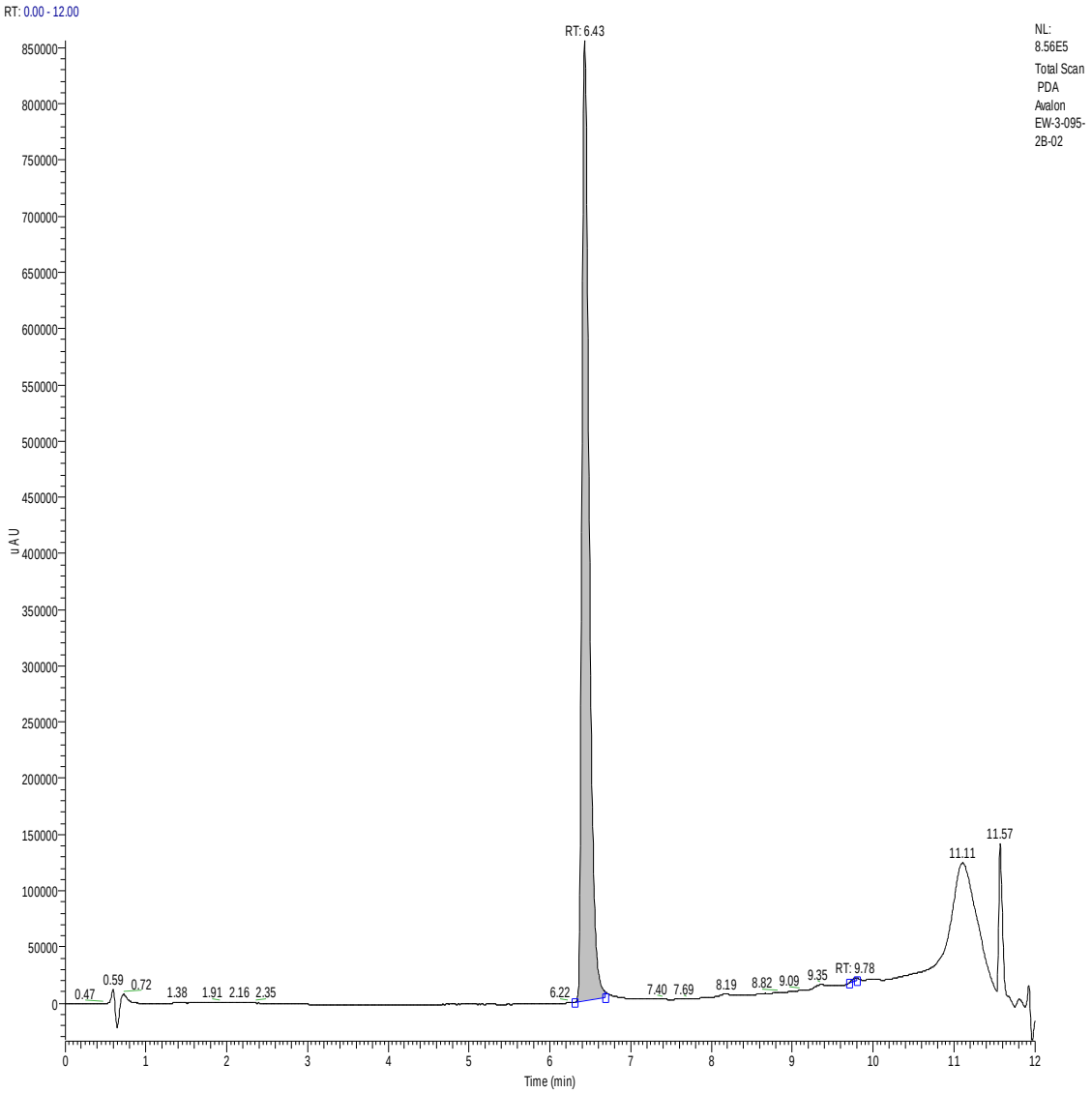


PEAK LIST

Compound 12a

Number of detected peaks: 3

Apex RT	Start RT	End RT	Area	%Area
4.99	4.93	5.08	9847.657	0.13
6.28	6.16	6.61	7396344.41	99.82
9.8	9.72	9.81	3652.944	0.05

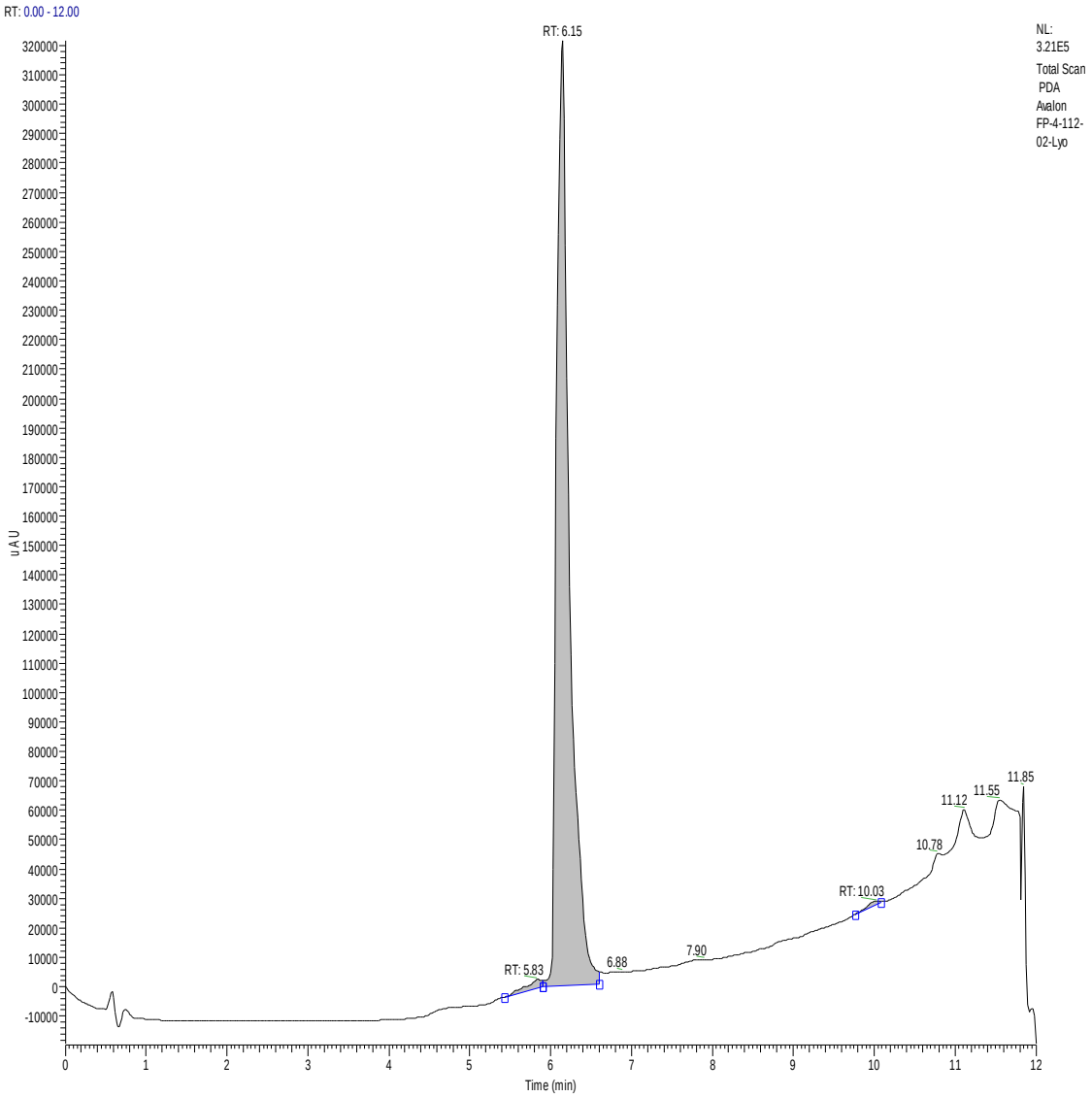


PEAK LIST

Compound 12b

Number of detected peaks: 2

Apex RT	Start RT	End RT	Area	%Area
6.43	6.31	6.68	5344603.39	99.84
9.78	9.71	9.8	8478.234	0.16

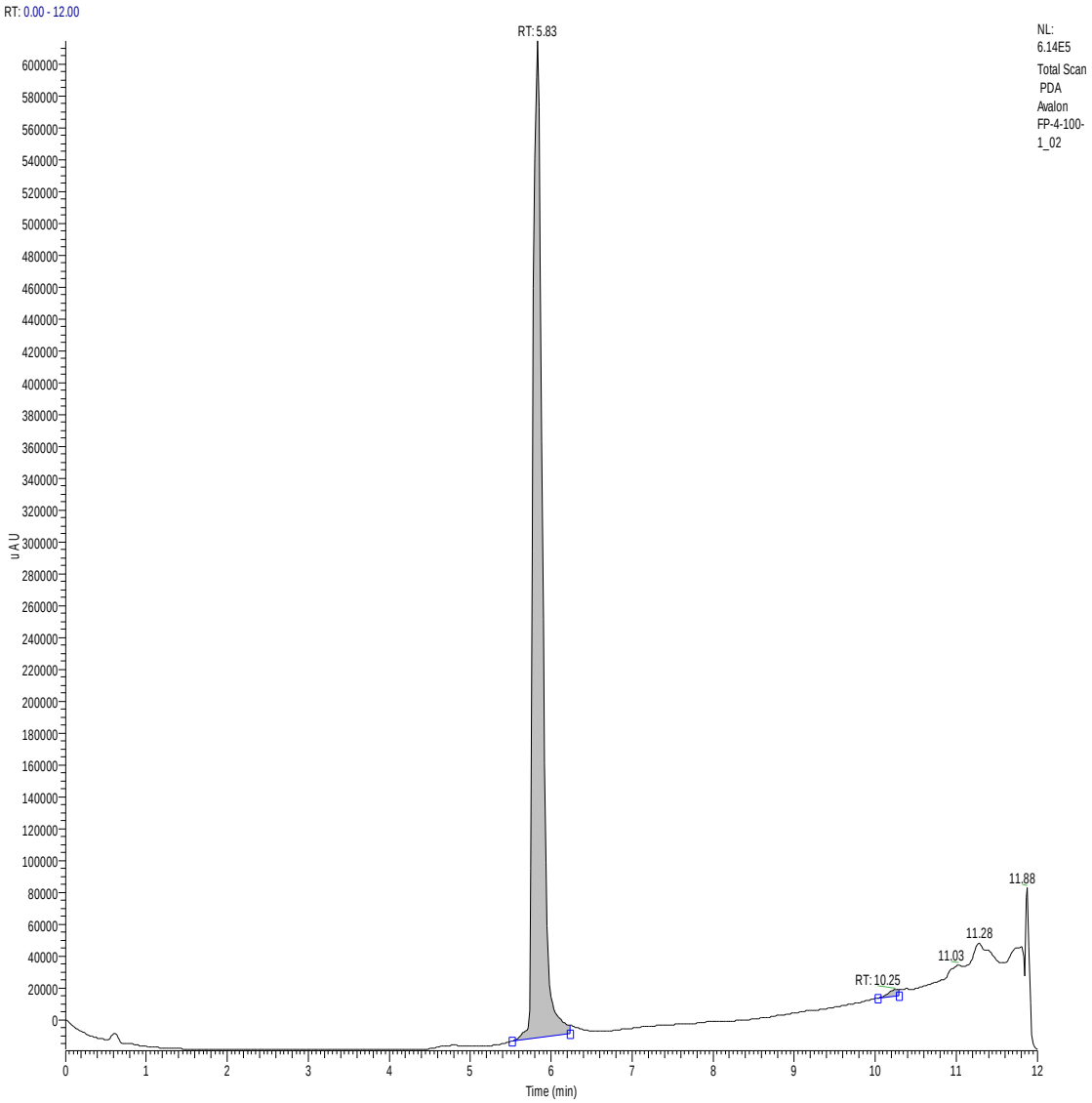


PEAK LIST

Compound 12c

Number of detected peaks: 3

Apex RT	Start RT	End RT	Area	%Area
5.83	5.43	5.9	43306.577	1.19
6.15	5.9	6.6	3588135.05	98.41
10.03	9.77	10.08	14652.897	0.4

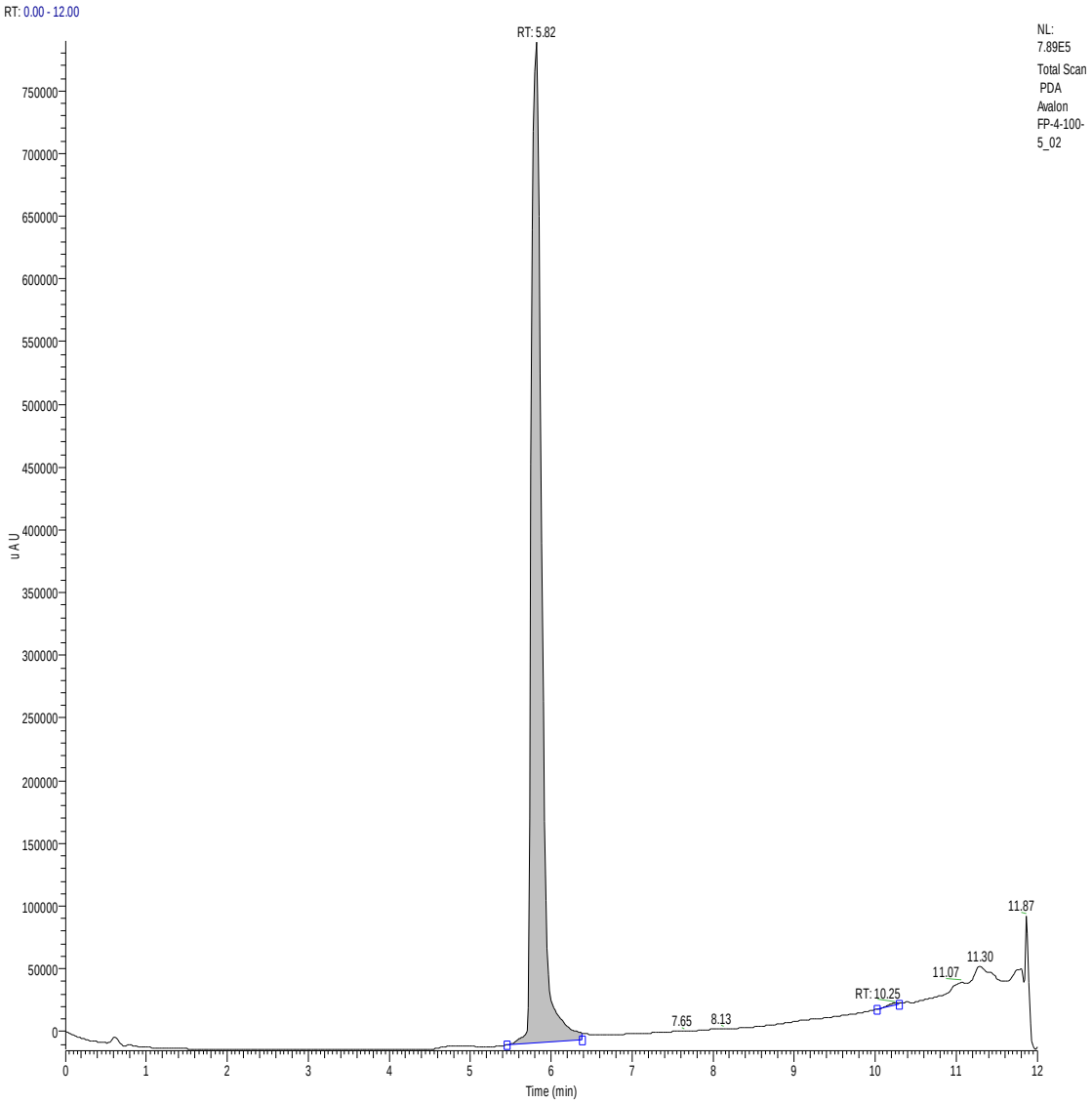


PEAK LIST

Compound 19a

Number of detected peaks: 2

Apex RT	Start RT	End RT	Area	%Area
5.83	5.52	6.23	5023906.3	99.37
10.25	10.03	10.3	31986.244	0.63

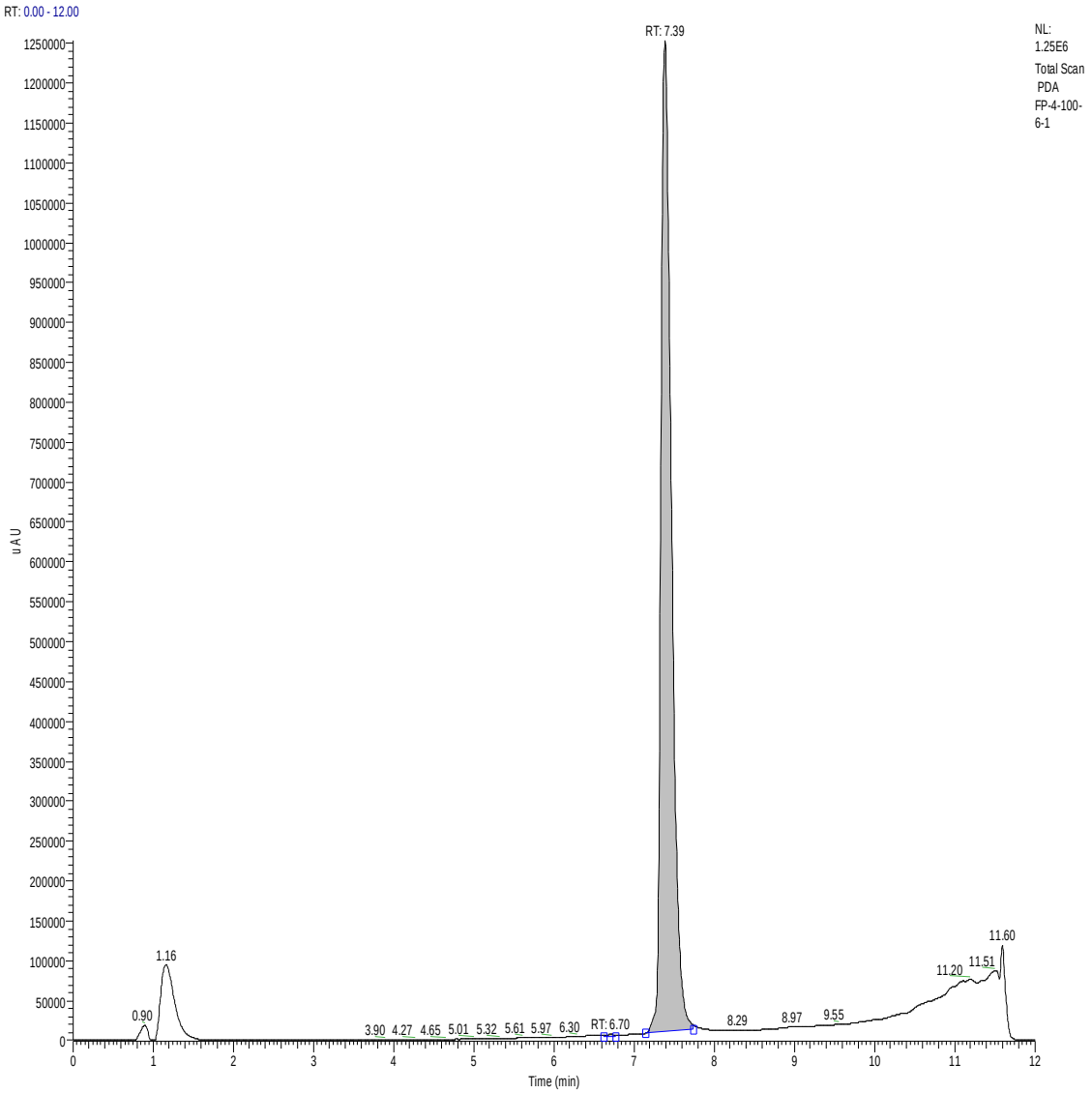


PEAK LIST

Compound 19b

Number of detected peaks: 2

Apex RT	Start RT	End RT	Area	%Area
5.82	5.45	6.38	7086167	99.75
10.25	10.02	10.3	17629.859	0.25

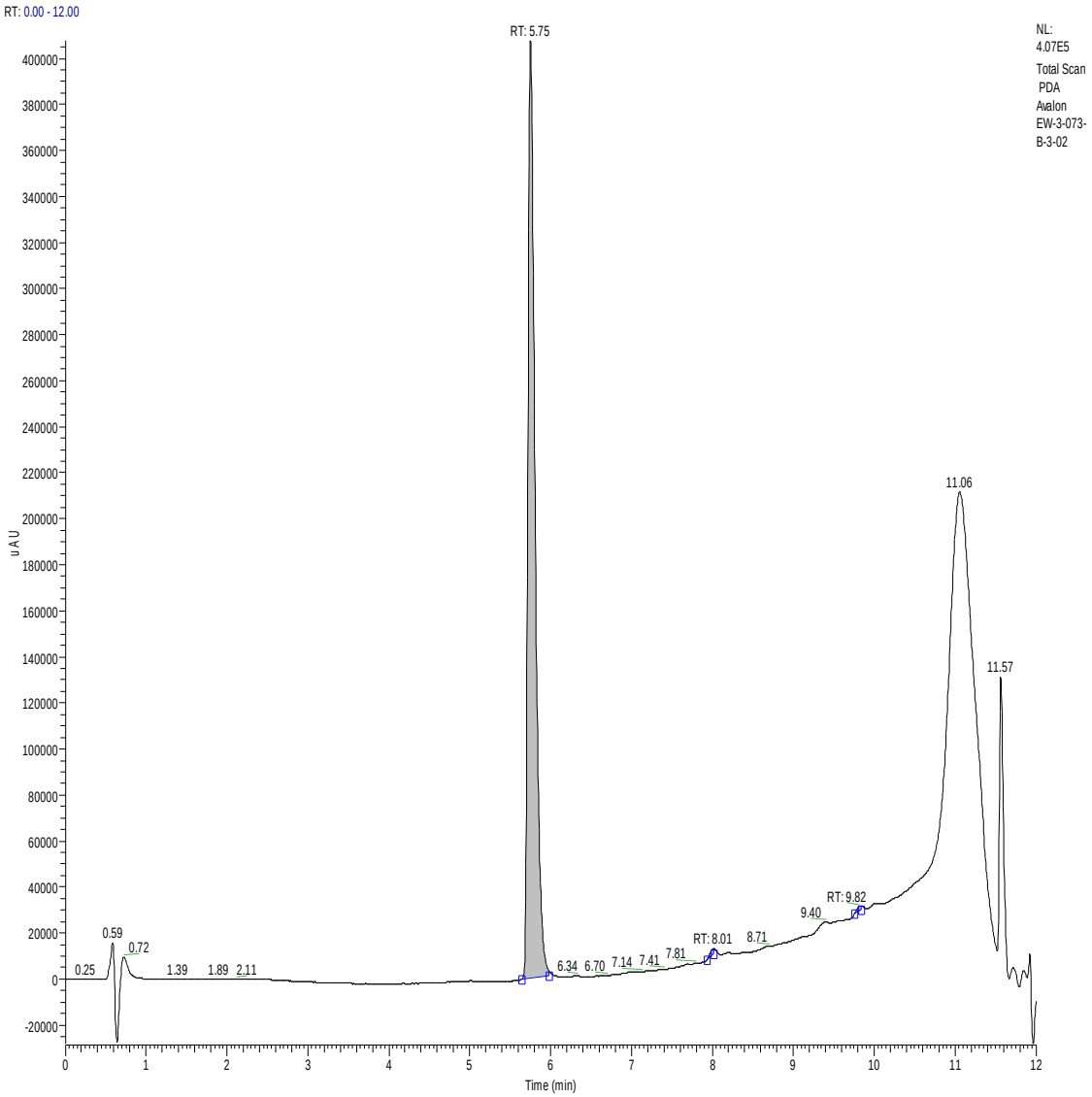


PEAK LIST

Compound 19c

Number of detected peaks: 2

Apex RT	Start RT	End RT	Area	%Area
6.7	6.62	6.77	14148.524	0.12
7.39	7.15	7.74	11344019	99.88

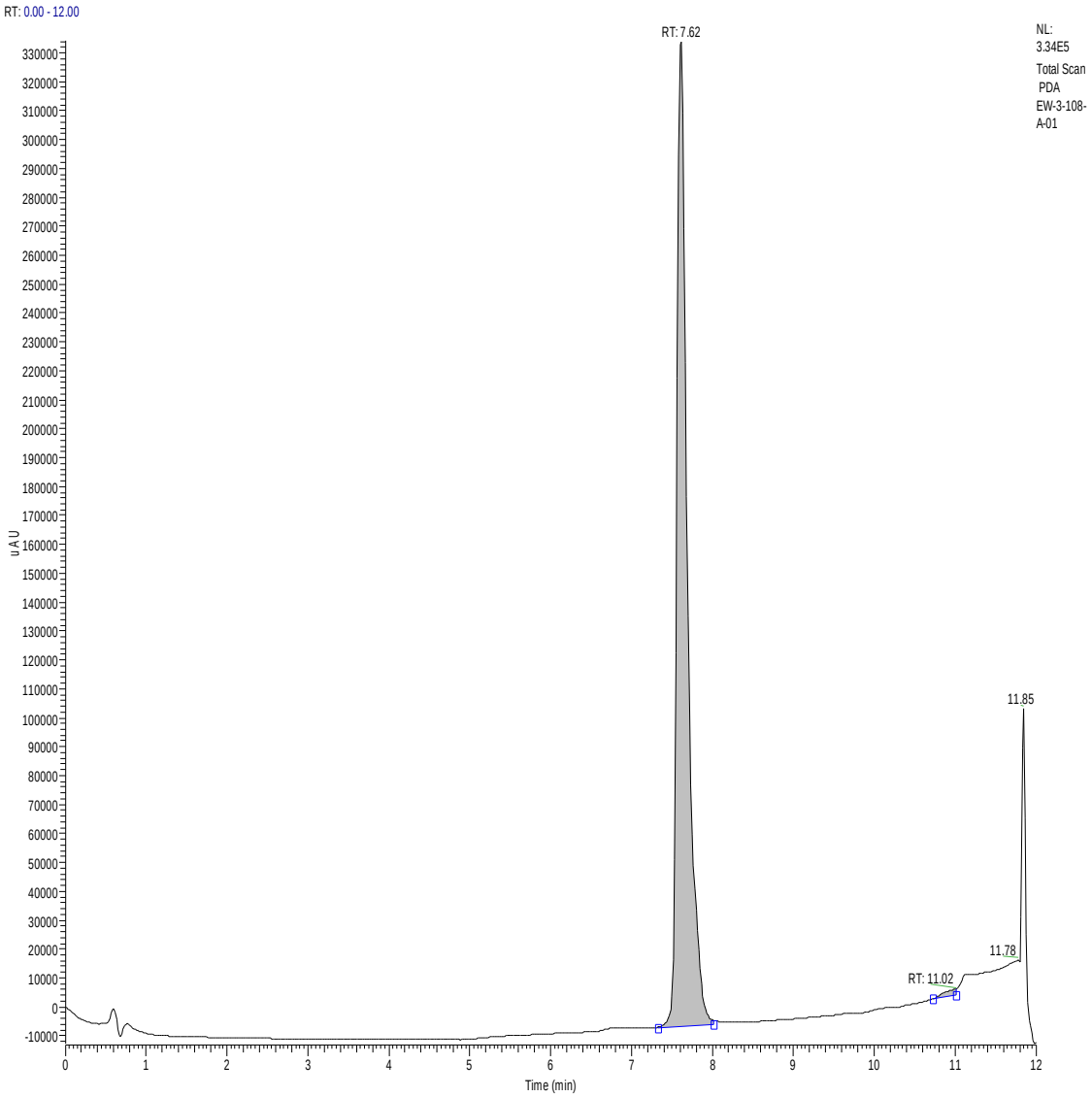


PEAK LIST

Compound 19d

Number of detected peaks: 3

Apex RT	Start RT	End RT	Area	%Area
5.75	5.65	5.98	2526804.22	99.38
8.01	7.93	8.02	9183.512	0.36
9.82	9.76	9.84	6618.061	0.26

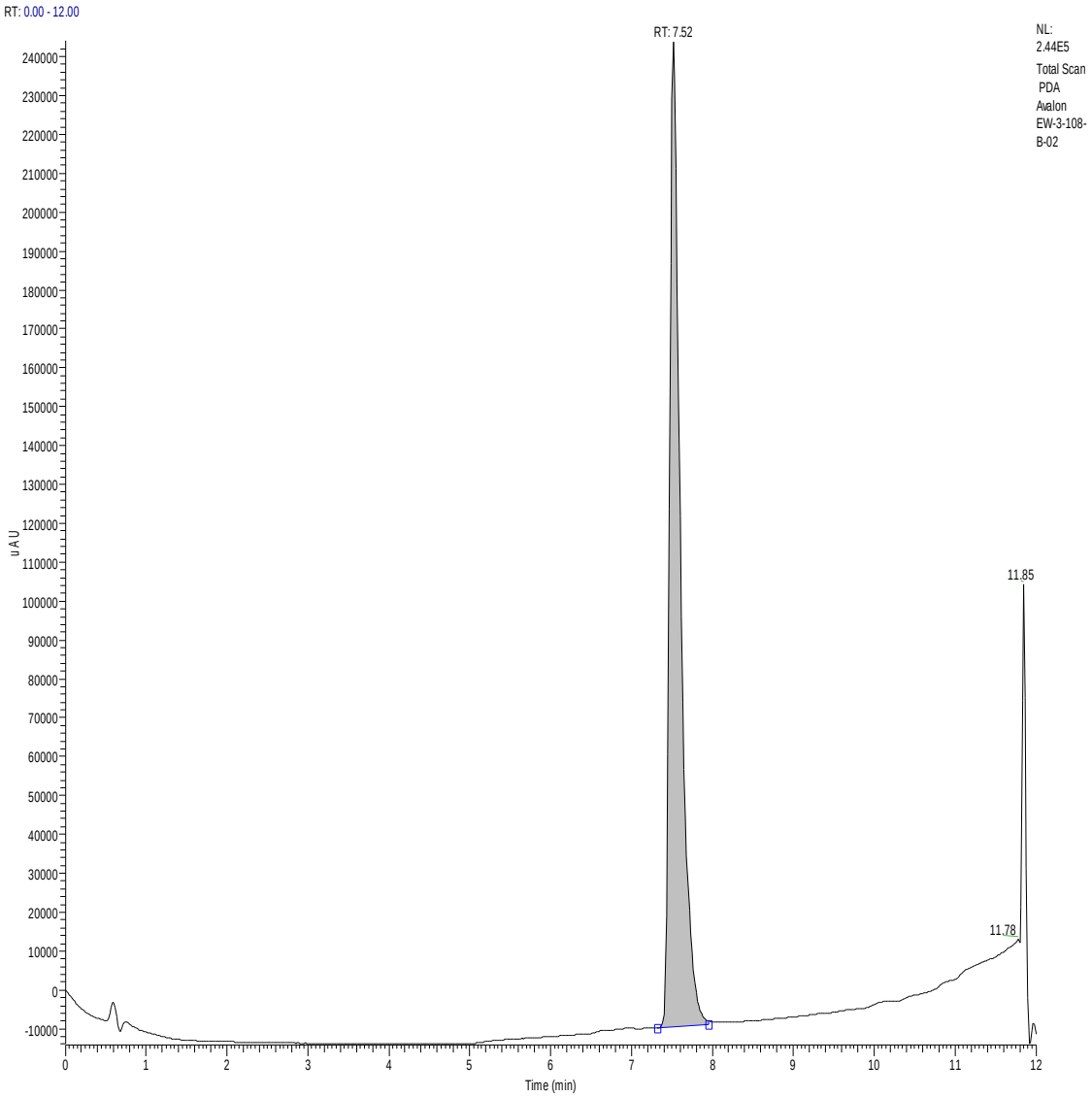


PEAK LIST

Compound 19e

Number of detected peaks: 2

Apex RT	Start RT	End RT	Area	%Area
7.62	7.33	8.02	3114185.62	99.28
11.02	10.73	11.02	22671.213	0.72

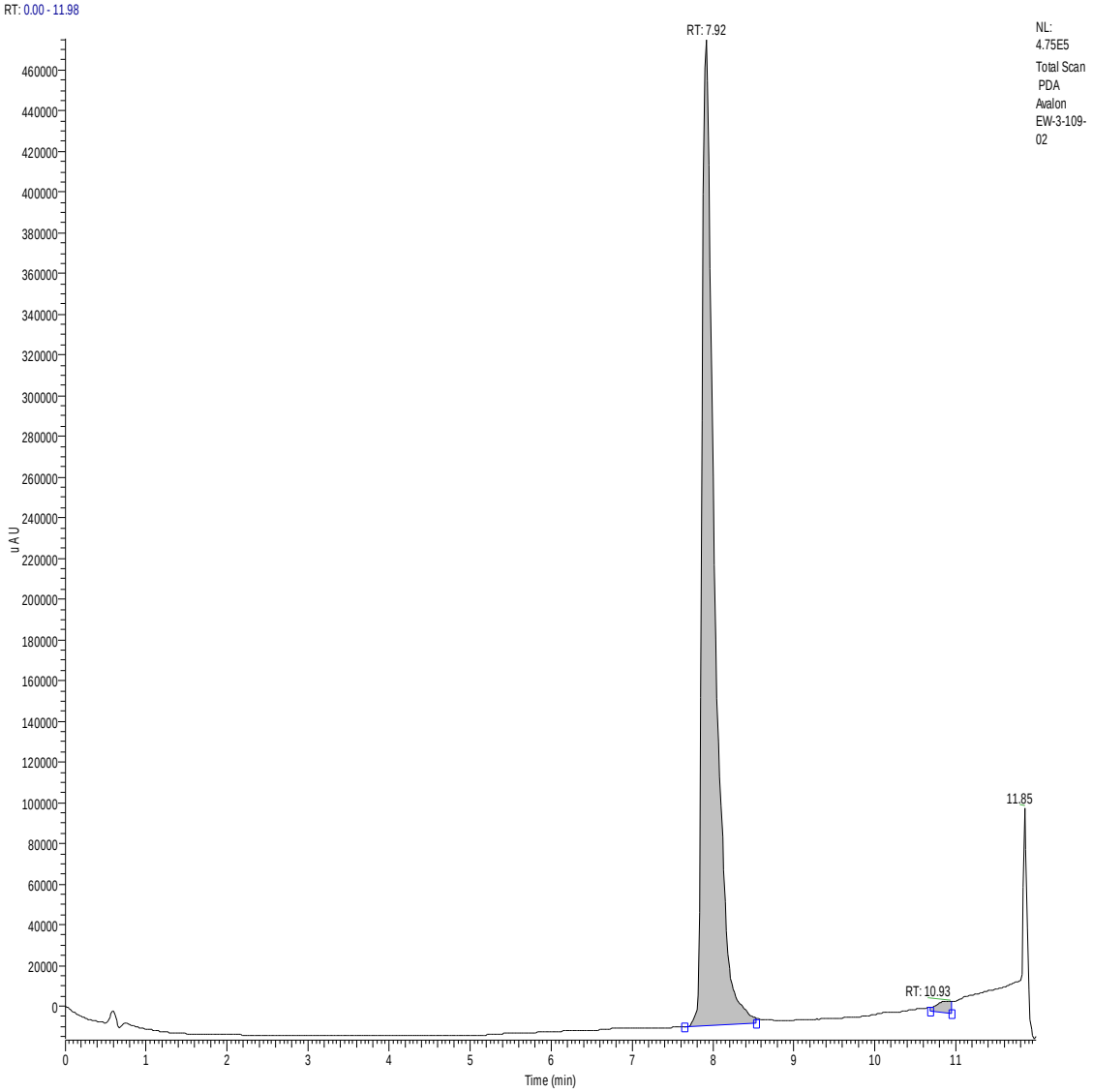


PEAK LIST

Compound 19f

Number of detected peaks: 1

Apex RT	Start RT	End RT	Area	%Area
7.52	7.32	7.95	2399711.49	100

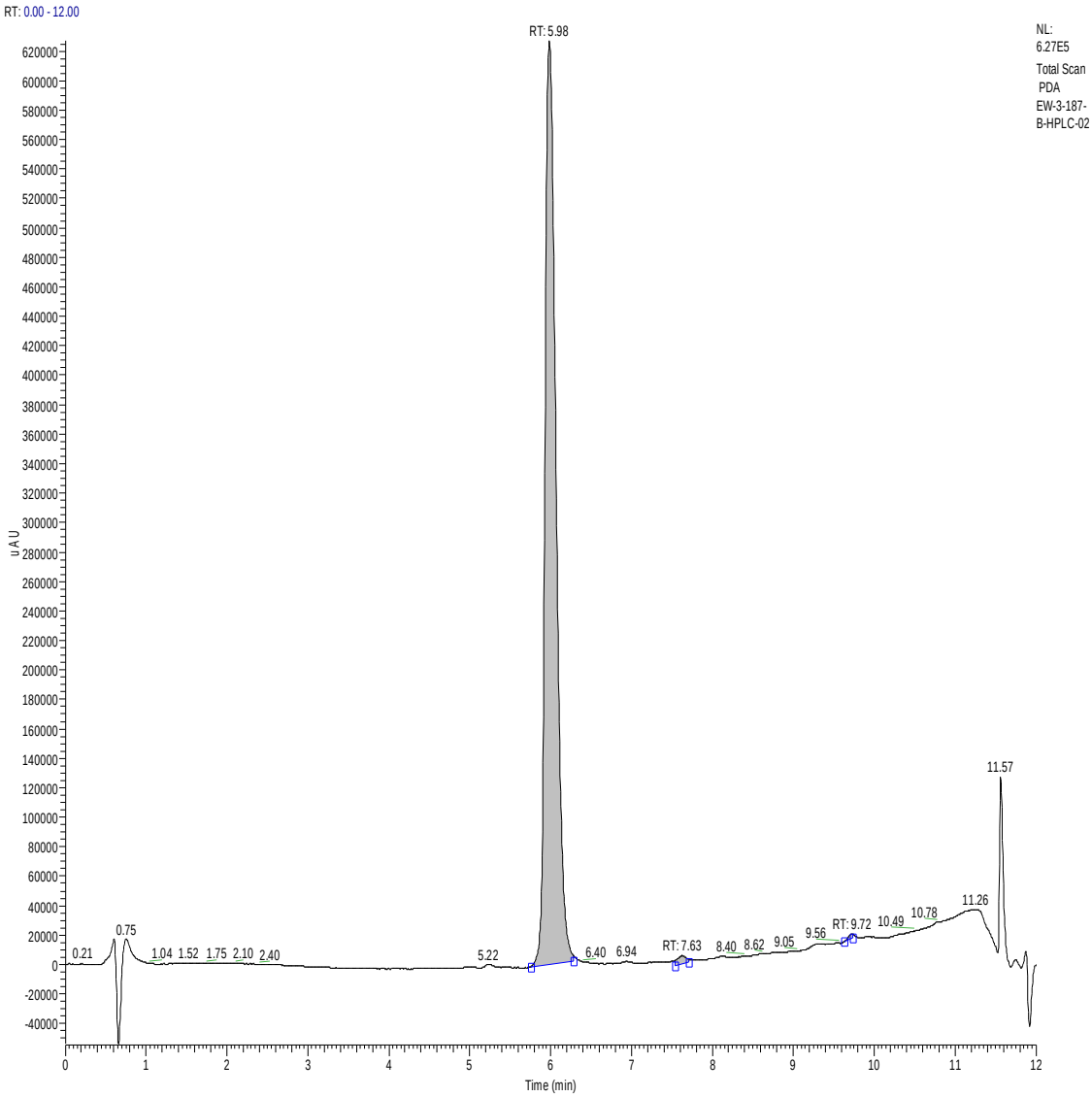


PEAK LIST

Compound 19g

Number of detected peaks: 2

Apex RT	Start RT	End RT	Area	%Area
7.92	7.65	8.53	5226563.23	98.68
10.93	10.68	10.95	69738.418	1.32

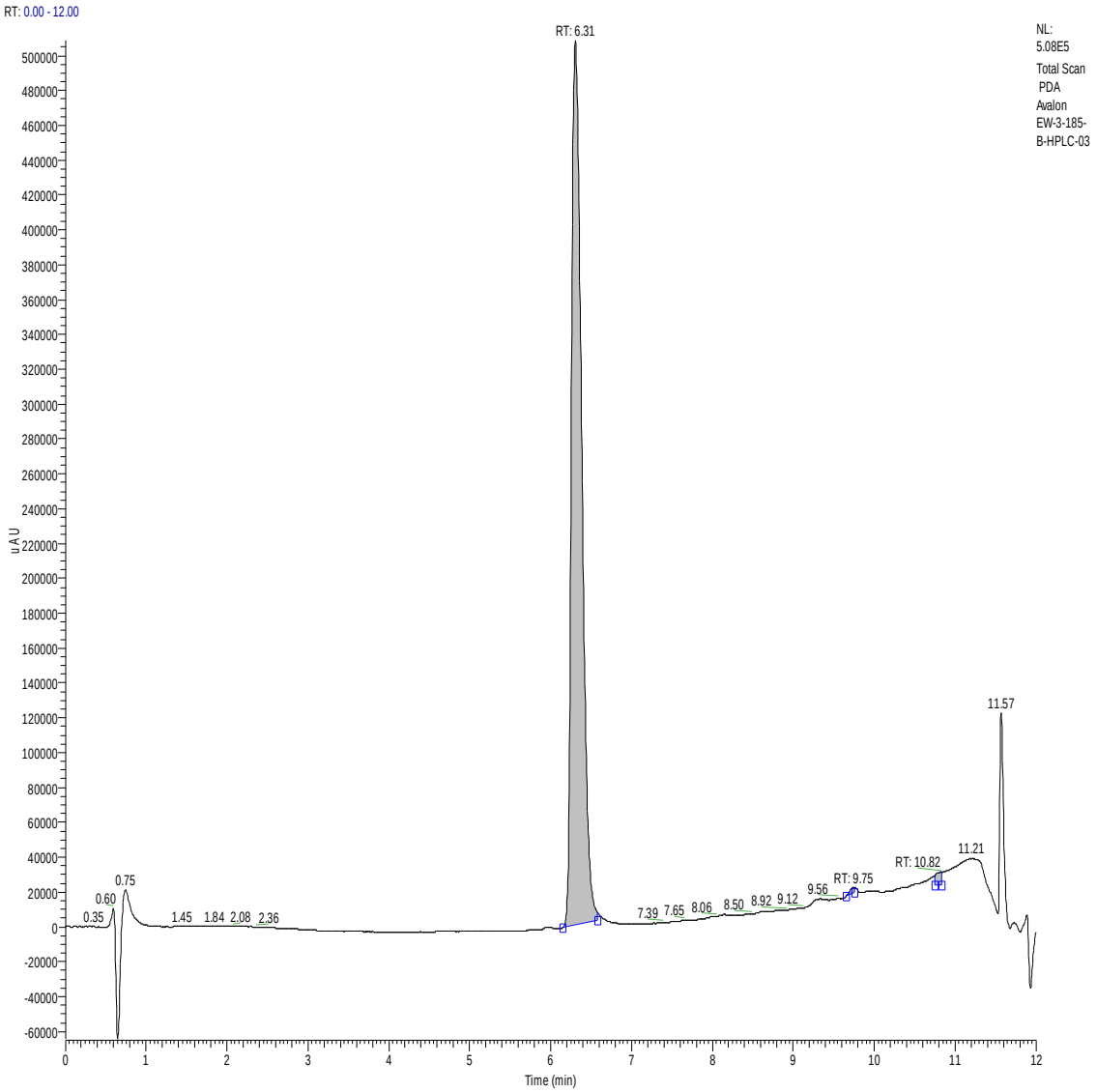


PEAK LIST

Compound 19h

Number of detected peaks: 3

Apex RT	Start RT	End RT	Area	%Area
6.31	6.15	6.58	4480803.34	98.91
9.75	9.65	9.76	12976	0.29
10.82	10.75	10.83	36419.203	0.8

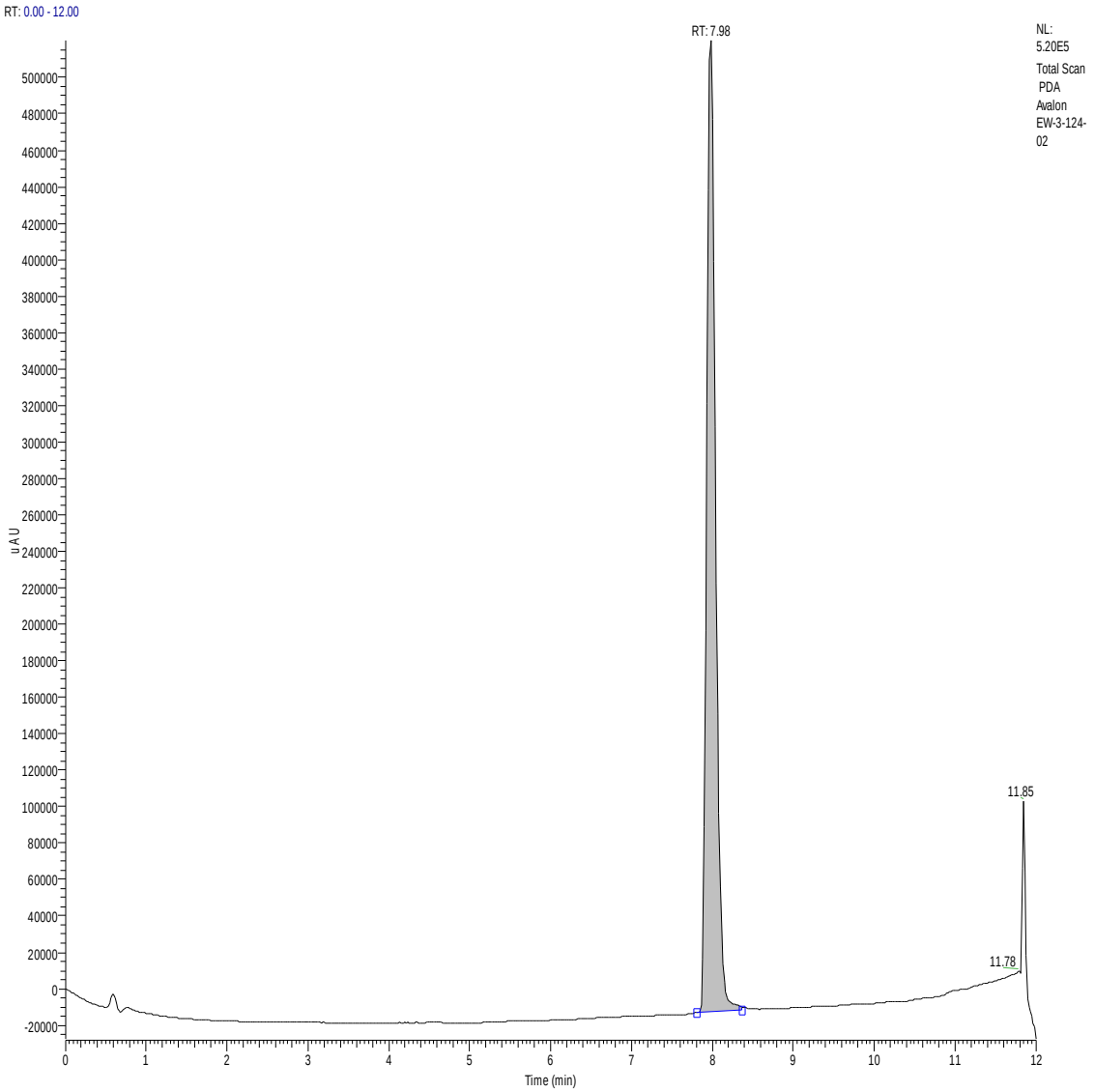


PEAK LIST

Compound 19i

Number of detected peaks: 3

Apex RT	Start RT	End RT	Area	%Area
5.98	5.76	6.29	5844873.86	99.06
7.63	7.54	7.71	44676.831	0.76
9.72	9.63	9.73	10679.424	0.18

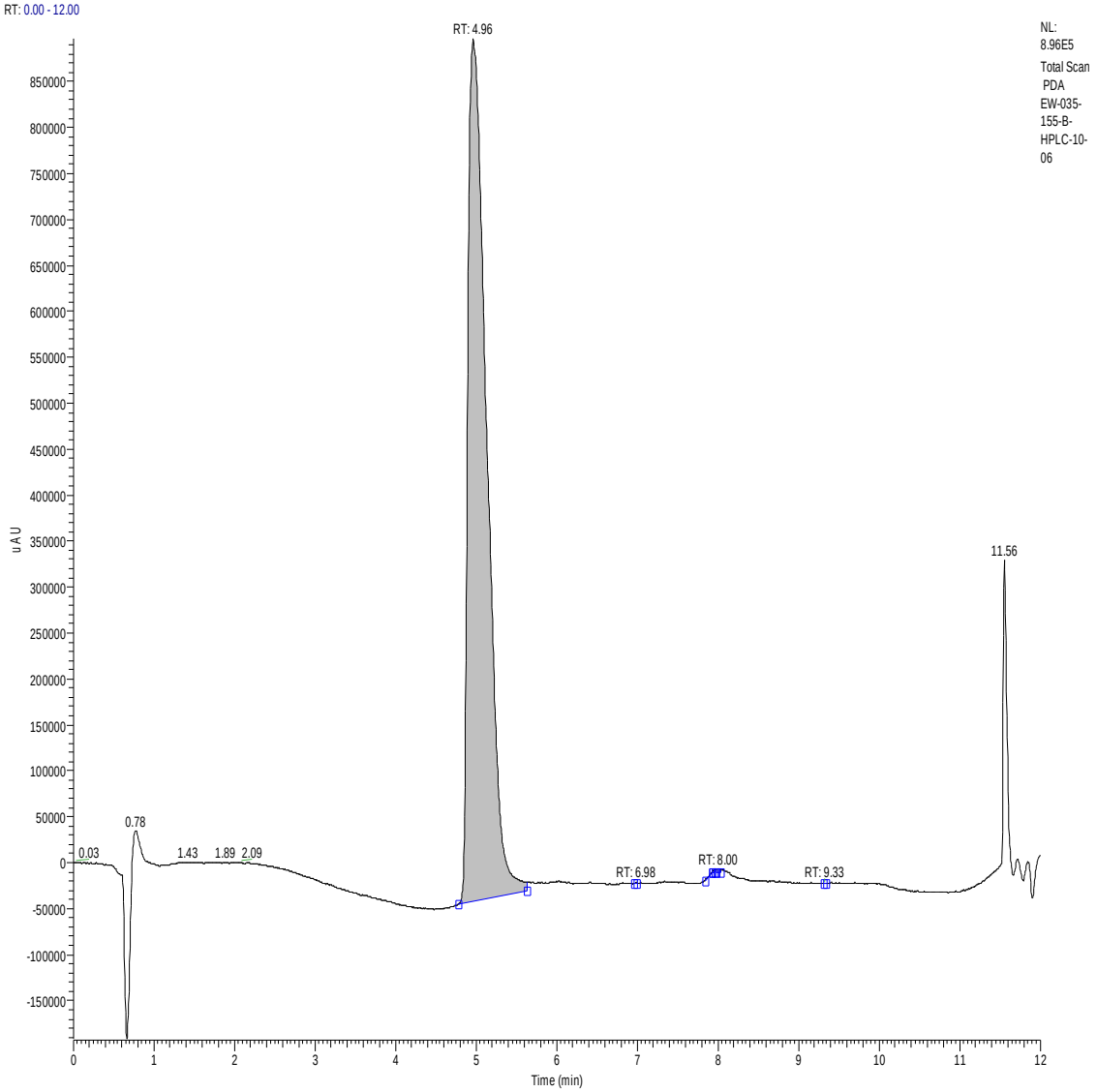


PEAK LIST

Compound 19j

Number of detected peaks: 1

Apex RT	Start RT	End RT	Area	%Area
7.98	7.8	8.37	4123075.99	100

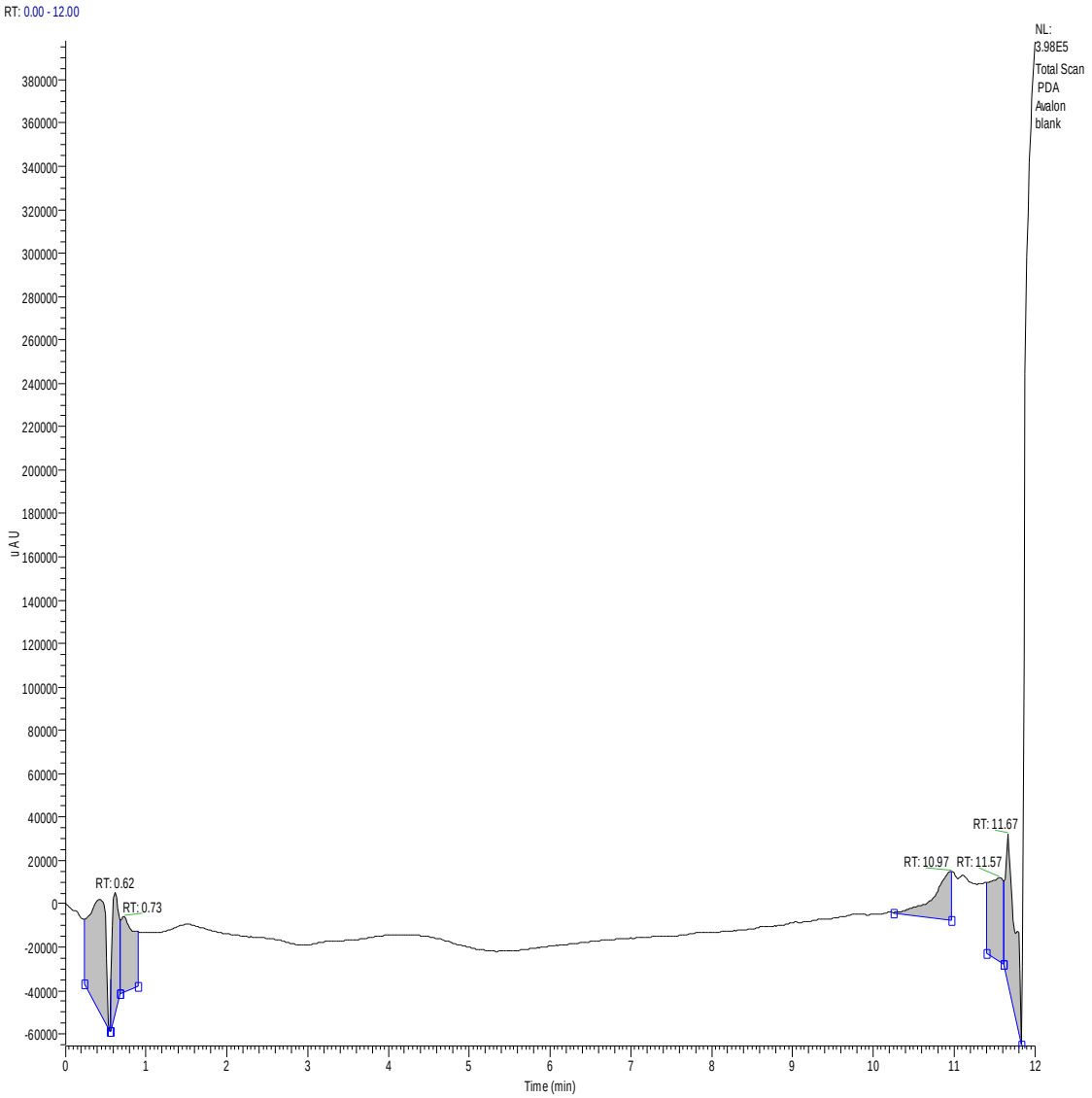


PEAK LIST

Compound 19k

Number of detected peaks: 6

Apex RT	Start RT	End RT	Area	%Area
4.96	4.78	5.63	15184092.4	99.82
6.98	6.97	6.99	587.519	0
7.92	7.85	7.93	5792.276	0.04
7.96	7.93	7.96	4324.893	0.03
8	7.98	8.04	15141.62	0.1
9.33	9.32	9.34	1000.287	0.01



Bank injection

PEAK LIST

Blank injection
(no compound)

Number of detected peaks: 6

Apex RT	Start RT	End RT	Area	%Area
0.43	0.23	0.55	765338.949	26.7
0.62	0.57	0.68	322062.405	11.23
0.73	0.68	0.9	386396.307	13.48
10.97	10.25	10.97	329396.857	11.49
11.57	11.4	11.62	472350.362	16.48
11.67	11.62	11.83	591081.934	20.62